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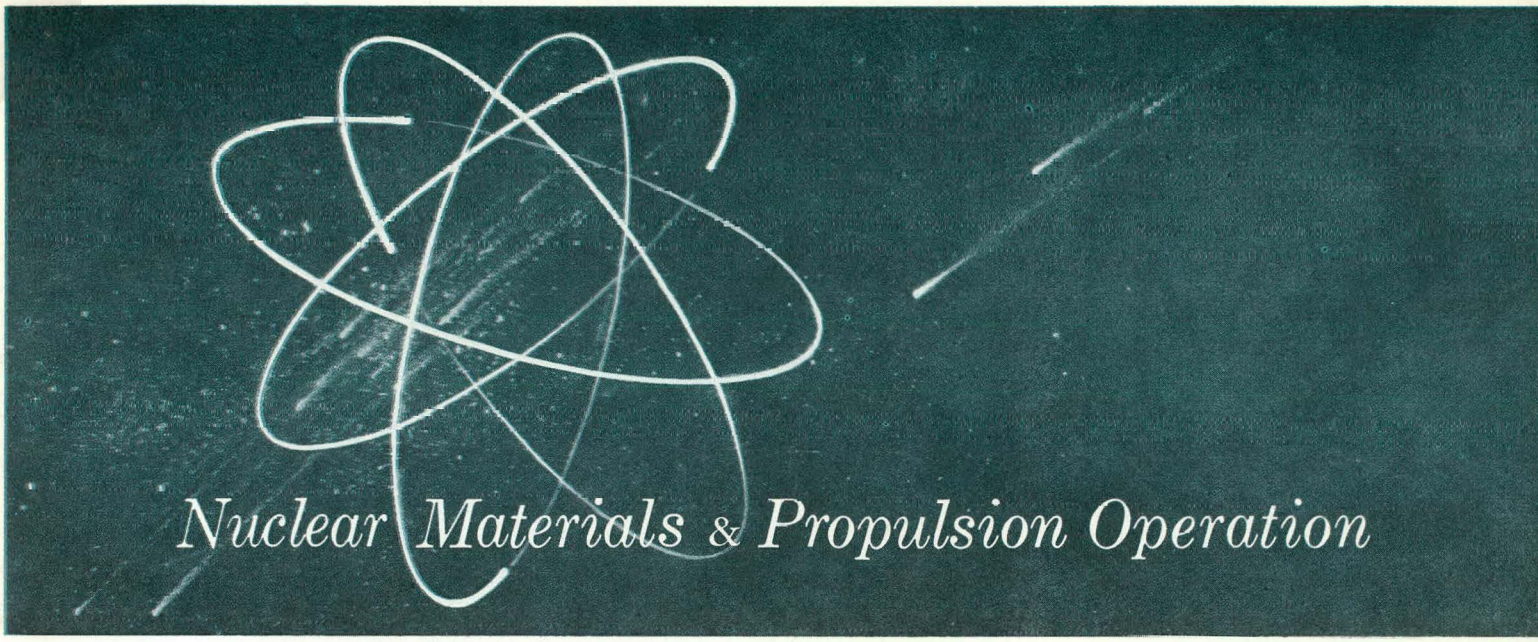

CASCADE and CLUSTER

Computer Programs
To Simulate Radiation Damage Processes In Metals
And Analyze The Distribution Of Defects

D. G. Besco and N. R. Baumgardt

April 1965

ADVANCED TECHNOLOGY SERVICES

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Clearinghouse for Federal Scientific
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5285 Port Royal Road
Springfield, Virginia 22151

GEMP-356
(INFORMAL)
UC-32, Mathematics
and Computers
TID-4500 (39th Ed.)

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United States Atomic Energy Commission Contract No. AT(40-1)-2847

NUCLEAR MATERIALS and PROPULSION OPERATION
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Table of Contents

I INTRODUCTION

Computational work has been performed as part of the radiation effects program at NMPO in an effort to describe (a) the dynamics of displacement cascades in the keV energy range in beryllium oxide and in metals, and (b) the resulting distribution of point defects and defect clusters. The published results from these studies may be found in references [1-5]. The computer programs used to provide data for (a) and (b) are called CASCADE and CLUSTER, respectively.

Since their conception, both these programs have been continually evolving. Improvements to the physical model have been made repeatedly as new theoretical and experimental data has become available, and the programs have been adapted and extended to various special purposes as new areas of investigation became of interest. Program reports exist for CASCADE for a square planar lattice version [6], a BeO version [7], and an early version for body-centered cubic and face-centered cubic lattices [8]. Since these reports were issued, CASCADE and CLUSTER have been combined into a single chain job, some new complexities have been introduced into the physical model, and some new options and extra features have been built in.

The purpose of the present report is three-fold:

(a) To provide a self-contained set of instructions (Chapter V) for using the combined CASCADE-CLUSTER program.

(b) To document CLUSTER (Chapters II, VI)

(c) To update reference [8] with respect to the additional program options, and the refinements which have been made to the model during the past year (Chapters III, IV).

II THE CLUSTER PROGRAM

Part of the output of CASCADE is a list of the coordinates of individual point defects produced in a displacement cascade: vacancies and interstitial atoms. This list may then be transmitted to CLUSTER for analysis.

CLUSTER performs three basic functions:

(a) Searches the lists of vacancies and interstitials for Frenkel pairs which are unstable, i.e. will immediately recombine, and removes these configurations from the defect lists.

(b) Having removed the unstable pairs, searches the lists for defects which by virtue of their position are members of aggregates: divacancies, di-interstitials, trivacancies, and clusters containing an arbitrarily large number of vacancies and interstitials. (For simplicity, all aggregates of two or more members are called "clusters", since they are treated logically in the same fashion). The individual members of each cluster are itemized, and a statistical breakdown of the number of each cluster type is printed.

(c) Computes distribution functions for the separation distance and minimum separation distance between various pairs of defect types.

There are two CLUSTER programs: one for b.c.c. and one for f.c.c.

1. Interstitial Configurations

The coordinate system used in the defect lists is one in which two units are equal to one lattice spacing, and (1,1,1) is a lattice site. This implies that the coordinates of a b.c.c. lattice site are integers and are either all even or all odd, and that the coordinates of an f.c.c. lattice

site are integers, and that their sum is odd. (ref. [8], section II.2). Motivated by symmetry considerations, the possible sites for interstitials in CASCADE are those positions which have integer coordinates and which are not lattice sites. These are the so-called "octahedral" interstitials in b.c.c. and "body-centered" interstitials in f.c.c.

Theoretical calculations have indicated, however, that the minimum energy configuration for a single interstitial in copper [9,10] is a "split" interstitial around a lattice site, oriented along < 100 >. Similarly, the most stable configuration in iron [11,12,13] is split around a lattice site, oriented along < 110 >.

Since CLUSTER has been used initially for iron and copper calculations, it assigns the interstitials generated by CASCADE to lattice sites for purposes of determining clustering and computing separation distances. An octahedral interstitial is assigned randomly to one of the two nearest lattice sites from which it is equidistant, and a body-centered interstitial is assigned randomly to one of the six nearest lattice sites from which it is equidistant.

2. Frenkel pair instability

The criteria for determining which Frenkel pairs (vacancy-interstitial pairs) are unstable are taken from references [9] (f.c.c.) and [12] (b.c.c.).

When an atom is ejected from a lattice site during a CASCADE calculation, it is considered to form a stable Frenkel pair if it comes to rest in an octahedral or body-centered interstice which is distant from its original lattice site by greater than $\sqrt{R}$ coordinate units, where R is an input variable usually set equal to 5. If the distance is less than $\sqrt{R}$, CASCADE performs a recombination.

However, CASCADE cannot sense close pairs which are due to an atom coming to rest less than $\sqrt{R}$ units from a vacancy which is not its own vacancy. Neither can it sense pairs which are separated by a distance greater than $\sqrt{R}$, but which are unstable due to their orientation along a close-packed line of atoms. CLUSTER does these things.

(a) B.c.c.

A Frenkel pair is unstable in b.c.c. if the members of the pair are first, second, or fifth neighbors, or if they are tenth neighbors separated by a close-packed < 111 > line of atoms. CLUSTER tags each recombination with a type number as follows:

	Relative Coordinates	Neighbor	Separation
Type 0	(000)	-	0
Type 1	(100)	-	1
Type 2	(111)	1	$\sqrt{3}$
Type 3	(200)	2	2
Type 4	(222)	5	$\sqrt{8}$
Type 5	(333)	10	$\sqrt{27}$

The program sorts for pairs of types 0 and 1 before assigning the octahedral interstitials to lattice sites. CASCADE may itself assign an interstitial to a lattice site if the target atom in a terminal (i.e., type 4) collision is itself an interstitial. This accounts for the existence of type 0 pairs.

(b) F.c.c.

A Frenkel pair is unstable in f.c.c. if the members of the pair are first, second, or fourth neighbors, or if they are ninth neighbors separated by a close-packed < 110 > line of atoms.

	Relative Coordinates	Neighbor	Separation
Type 0	(000)	-	0
Type 1	(100)	-	1
Type 2	(110)	1	$\sqrt{2}$
Type 3	(200)	2	2
Type 4	(220)	4	$\sqrt{8}$
Type 5	(330)	9	$\sqrt{18}$

3. Defect Clusters

(a) B.c.c.

In iron, the most stable divacancy is the one in which the vacancies are at second neighbor lattice sites [13]. CLUSTER therefore records a vacancy pair as a divacancy if the separation is either first or second neighbor, and itemizes the two cases separately.

By extension, a cluster of n vacancies in b.c.c. is defined to be a set of n vacancies such that each vacancy in the set has a first or second neighbor which is also in the set. For the purpose of cluster formation, each lattice site has 14 neighbors: 8 first and 6 second.

The most stable di-interstitial in iron consists of two split interstitials parallel to each other at first neighbor lattice sites [13]. CLUSTER therefore requires first neighbor separation before two interstitials are considered to be a di-interstitial. Similarly for higher order interstitial clusters.

(b) F.c.c.

The first neighbor divacancy is stable in copper [14]. Therefore, a cluster of n vacancies in f.c.c. is defined to be a set of n vacancies such that each vacancy in the set has a first neighbor which is also in the set. The neighbors of a vacant lattice site for the purpose of cluster formation are therefore its 12 first neighbors.

4. Distance between Clusters

For the purpose of computing distance distributions, CLUSTER classifies the defects into six categories:

1. single vacancies
2. divacancies
3. immobile vacancies
4. single interstitials
5. di-interstitials
6. immobile interstitials

All clusters with three or more members are called "immobile".

For each pair (i,j) of defect types, CLUSTER produces a distance table. There may be a maximum of 21 tables ($i \leq j$), in the case where there is more than one of each defect type.

Suppose there are N_i defects of type i and N_j defects of type j. The distance between every (i,j) pair is computed. If $i \neq j$ the number of distances is $N_i N_j$. If $i = j$, the number of distances is $\frac{N_i(N_i-1)}{2}$. A histogram and cumulative distribution are computed. For the purpose of computing distances, the position of a cluster is taken to be the centroid of the set of single defects composing the cluster.

Also, for each defect of type i, the distance to the nearest defect of type j is computed. The number of distances is always N_i. Again, a histogram and cumulative distribution are calculated.

A more complete description of the distance tables is given in Chapter VI.

III THE CASCADE PROGRAM

Reference [8] was the original program report for the b.c.c.-f.c.c. version of CASCADE. Chapter II of that report (Physical Model and Computation Methods) is still an accurate description, and the information from that chapter is not repeated in this report. The present chapter serves as an addendum, describing the additional capabilities which have been incorporated into the program.

Chapters III and IV of reference [8] (Program Usage and Programming Information) are to a considerable extent obsolete, and they are updated by this report.

1. Saturation

Studies of the saturated damage state may be made using the feature of CASCADE which allows the damage pattern which CASCADE creates and from which CLUSTER removes the unstable Frenkel pairs, to be used as the initial damage state for a new CASCADE run. This process may be repeated as many times as desired.

Although similar calculations could be done with the original program, the new feature represents a considerable improvement to the physical model, in that all unstable configurations are removed at each step of the way.

The procedure for making saturation runs is now fully automated, requiring very little preparation of data by hand. Details are given in Chapter V.

2. Minor improvements to the calculation method

a) Temporary interstitials

When an interstitial atom was displaced from an interstice, the earlier program printed a message to this effect, indicating the necessity for hand

alteration of the defect list. This condition is now handled automatically by the program, and no message is printed.

b) Relaxation parameter

As indicated in section II.2, the initial criterion that the displacement of an atom from a lattice site be "permanent", is that the displaced atom replaces another atom at a lattice site, or comes to rest in an interstice greater than $\sqrt{R}$ from the site it vacated.

c) Replacement collisions

At the user's option, the program will either record all replacement collisions, or record only those which would disorder a binary crystal.

d) Tracing method

The f.c.c. tracing routine has been slightly modified. The forbidden targets in a collision search are the last n atoms struck by the moving atom, where n is the number of grazing ($p > 1$ Å) collisions which that atom has had. If $n > 3$, n is taken to be 3.

IV PROGRAMMING INFORMATION

1. System and setup

CASCADE and CLUSTER are coded in FORTRAN II and FAP. Together they make up a chain job consisting of either three or four chain links, depending upon the problem. Execution is under control of the FORTRAN Monitor System.

The programs use subroutine FNBTP [15] to read and write binary tape. This subroutine may write physical records longer than 458 words, which makes the program incompatible with the IBM Direct Couple Operating System [16]. Therefore, the program may not be executed on directly coupled 7094/7040 configurations, such as the one at Wright-Patterson Air Force Base, until the binary tape I/O is recoded.

The symbolic tape units addressed by the program are the following:

2 - BCD input

3 - BCD output

5 - Occupancy change tape (binary)

7 - Defect list tape (binary)

10 - Potential data tape (binary)

13 - Saturation tape (binary)

Tapes 10 and 13 are specific reels mounted prior to execution. Tape 5 is a scratch tape. Tape 7 is a binary output tape which should be saved after any production runs involving several change cases, at least until it is known whether there were data or other errors that caused the job to be terminated prematurely.

2. Program organization

For a normal CASCADE-CLUSTER job there are three chain links, as follows:

CHAIN (1,B2)	CASCADE link
CHAIN (1,B3)	EDIT link
CHAIN (2,B3)	CLUSTER link

For each case, CASCADE is executed once, then EDIT is executed once. These two links are executed alternately until all cases have been run. At that time, CLUSTER is called in, and processes all cases. CLUSTER is loaded just once for each job.

The output on tape 3 is in two parts: first the CASCADE printout for all cases, then the CLUSTER printout for all cases.

For a saturation job, a fourth chain link:

CHAIN (2,B2) SATURATION link

is added at the beginning of the binary deck. There is no provision for running saturation change cases, so in such a job each link is executed once.

3. Occupancy change tape

For every collision which changes the occupancy of a site, four words are written on tape 5 by the CASCADE link.

Let K = the atom type involved (1,2, or 3). Set N according to the following scheme:

N = 10: ejection from a lattice site

N = 20: tentative interstitial formation

N = 30: replacement collision

N = 40: recombination of a tentative interstitial with an ejection site.

N = 50: displacement from an interstice

Word 1 is equal to N + K, and words 2, 3, and 4 are equal to the lattice coordinates of the event.

Records of length 100 words (25 events) are written on tape 5 by the CASCADE link. The EDIT rewinds the tape after each case, reads it back into core, and produces the CASCADE defect list by examining each displacement event in sequence.

Tape 5 is also used to store the occupancy table prepared by the SATURATION link, for later use by the CASCADE link.

4. Defect List Tape

Tape 7 is the means of communicating the defect list from CASCADE to CLUSTER.

Let NVAC (J), J = 1, 2, be the number of vacancies of type J. Similarly, let NINT (J) be the number of interstitials.

Let KVACX (I,J) be the lattice coordinate in the X direction for the Ith vacancy of type J, I = 1,..., 500, J = 1, 2. Similarly for KVACY, KVACZ, KINTX, KINTY, KINTZ.

For each case, the EDIT link writes one record on tape 7. The

number of words in the record is

$$25 + 3(NVAC(1)+NVAC(2)+NINT(1)+NINT(2))$$

The format of the record is as follows:

Words 1-20: identification
Word 21: lattice constant
22: NVAC(1)
23: NVAC(2)
24: NINT(1)
25: NINT(2)

followed by the defect list:

KVACX (I,1), I = 1, NVAC(1)

KVACY (I,1), I = 1, NVAC(1)

KVACZ (I,1), I = 1, NVAC(1)

KVACX (I,2), I = 1, NVAC(2)

KVACY (I,2), I = 1, NVAC(2)

KVACZ (I,2), I = 1, NVAC(2)

KINTX (I,1), I = 1, NINT(1)

KINTY (I,1), I = 1, NINT(1)

KINTZ (I,1), I = 1, NINT(1)

KINTX (I,2), I = 1, NINT(2)

KINTY (I,2), I = 1, NINT(2)

KINTZ (I,2), I = 1, NINT(2)

One record is written on tape 7 for each case in the job. After the CASCADE calculations are complete an end of file is written, the CLUSTER link is loaded, rewinds 7 and uses it as an input tape, processing one record at a time until the end of file is encountered. When the end of file is read a message to that effect is printed, and tape 7 is rewound and unloaded before EXIT is called.

5. Potential Data Tape (collision matrix)

A table of energy transfers and scattering angles as functions of energy and impact parameter, corresponding to a given interatomic potential function [17], may be calculated and punched on decimal cards by the Collision Matrix Program (NMPO Program 770).

These cards may be included with the BCD card input each time. Alternatively, they may be used to prepared a binary data tape which is then mounted as tape 10 prior to each run.

The format for the potential data tape is as follows:

Record 1 - 2 words

Word 1: NE (Number of energy values)

Word 2: NIP (Number of impact parameter values)

Record 2 - NE+NIP+2*NE*NIP words

(E(J), J = 1, NE) energies

(P(I), I = 1, NIP) impact parameters

((COSINE (I,J), I = 1, NIP), J = 1, NE)

cosines of center-of-mass scattering angles.

((ETRA (I,J), I = 1, NIP), J = 1, NE)

energy transfer fractions.

Two data tapes are on file in the computer lab at Evendale. Reel number 3219 corresponds to Potential II for copper, of Gibson et al. [9]. Reel no. 4332 corresponds to Potential III for iron of Erginsoy et al. [12].

6. Saturation tape

Tape 13 is the means of communicating a CLUSTER defect list to a subsequent CASCADE.

When directed to do so by the input control word KSATUR (see input data instructions), the CLUSTER link writes on tape 13 the defect list which it received from CASCADE via tape 7, but with the unstable Frenkel pairs deleted.

The interstitials on tape 13 are on their original sites (octahedral or body-centered), rather than the lattice sites to which they are assigned by CLUSTER, because the tape subsequently provides CASCADE with an initial damage state. The tape is read by the SATURATION link, which uses the information to prepare an occupancy table. Later it is used by the EDIT link, which combines the information with that on the occupancy change tape, to produce a new defect list.

7. Error procedures

If an error condition occurs during CASCADE (including DING errors), the usual procedure is to print out an error message via a call to ERRORA, and then call subroutine EREX, which follows one of two exit procedures.

If the input specified that CLUSTER was to be run following CASCADE, EREX writes an end of file on tape 7, rewinds, sets location 77462_8 to non-zero as a signal to CLUSTER that the job terminated prematurely, and calls CLUSTER.

If CLUSTER was not specified, EREX simply rewinds and unloads tape 7, and calls EXIT.

There are two exceptions to this procedure. If a tape or other error is detected by a FORTRAN I/O subroutine, a message is printed and EXIT is called, with no opportunity for action by the program to salvage anything.

It is for this reason that tape 7 should be saved. The second exception is when a necessary data item is omitted from the first CASCADE case. In this situation, a message is printed and EXIT is called.

When CLUSTER is called by EREX, the spacing of tape 2 is indeterminate, so CLUSTER is unable to read input from tape 2. Instead, it uses values which are built in for such an emergency. It will process as many defect lists from tape 7 as were written correctly before the error occurred.

BTERR is a subroutine which is called after every usage of FNBTP. If an error was detected reading or writing binary tape, BTERR prints an appropriate error message.

8. Program limitations

The following limitations are imposed upon CASCADE by the amount of core storage available.

Item	Maximum number
Vacancies	500 of each type
Interstitials	500 " " "
Replacements	300 " " "
Primary knock-on atoms	300 " " "
Moving atoms	300 at any one time
Occupancy change events	3800
Damaged "boxes"	1500 (24,000 atoms in b.c.c., 48,000 in f.c.c.)

The program terminates a case automatically after 20,000 collisions (10,000 if only the primary atom is being traced).

9. Note on binary materials

The original CASCADE program was coded for a binary (AB) alloy. This is the reason for "Type A" and "Type B" atoms. However, computer limitations prevented several of the later additions from being fully general. For example, the collision matrix would require five times as much memory in the general case of an AB alloy being bombarded by a foreign atom. Also the CLUSTER procedure would be enormously complicated both physically and computationally if a disordered binary crystal were permitted. CLUSTER and SATURATION have therefore been coded only for the monatomic case.

Binary alloys, therefore, may be handled using only those options present in the original program. That is, a Bohr potential is used, and CLUSTER and SATURATION may not be used.

10. Program listings

The listing of the FORTRAN-FAP source deck for CASCADE-CLUSTER is not included in this report, because it is 175 pages long. Anyone interested should contact one of the authors.

11. Running the program at outside installations

The program, in one version or another, has been successfully run on 7090's and 7094's at Brookhaven National Laboratory, Oak Ridge National Laboratory, and Wright-Patterson Air Force Base (before the Direct Couple System), as well as at G.E.-Evendale.

Two items should be noted when not running under the Evendale system.

(a) Tape assignments

At Oak Ridge, logical-physical tape correspondences may be specified on control cards. Elsewhere, patches to the IOU table may be necessary, depending on the local system.

(b) Evendale library subroutines

Care should be taken that the Evendale library subroutines which are not part of the FORTRAN Monitor System as distributed by IBM, are included in the binary deck.

SATURATION link:	FNBTP
	DING
	ERROR
	(FPT)
	UNLOAD
CASCADE link:	ATAN
	ERROR
	EXP (3
	DING
	(FPT)
	SQRT
	UNLOAD
EDIT link:	(FPT)
	FNBTP
	UNLOAD
CLUSTER link:	DING
	ERROR
	FNBTP
	(FPT)
	SQRT
	UNLOAD

The mathematical subroutines (ATAN, EXP (3, SQRT) must be in the deck to insure uniformity of results to all decimal places, independent of where the program is run.

12. Running time

The approximate total running time on the 7090 for CASCADE-CLUSTER together is given below. The table is for copper, but other metals are of the same order, depending on such parameters as ejection energy and potential.

It is assumed that a collision history is to be printed out, which increases the running time. For the lower energies, it is assumed that there are many cases per run.

In some metals, particularly iron, the possibility of channeling makes the running time more unpredictable.

E(keV)	Min:sec/case
0.5	0:15
1.0	0:20
2.5	0:35
5	1:15
10	2:30
15	4:15
20	7:30

V INPUT DATA

This chapter is a self-contained set of instructions for running CASCADE and CLUSTER.

The input data is loaded by DING from tape 2.

Consider the simplest possible case, in which a single cascade is to be simulated in an initially perfect crystal, followed by the removal of unstable configurations and analysis of the damage pattern.

The required data items are discussed in sections V.1 and V.2. An example of the deck setup is given in V.3, and the numerous options and extensions are discussed in V.4.

1. Minimum Data (CASCADE)

(a) Case identification

Symbols: ID1 (10 words), ID2 (10 words)

Two lines of Hollerith identification. They appear on the first page of the CASCADE printout and on every page of the CLUSTER printout.

(b) Atom identification

Symbols: TYPE 1 (2 words), TYPE 2 (2 words), TYPE 3 (2 words)

Hollerith names of type A atom, type B atom, and primary atom, respectively.

(c) Crystal structure identification

Symbol: CRYSTL (one word)

Hollerith name of crystal structure. Either "BCC" or "FCC".

(d) Atom parameters

Symbols: PCHG, PMASS, ED, (3 words each: type A, type B, and primary)

PCHG = atomic number

iron: 26

copper: 29

tungsten: 74

PMASS = mass number

iron: 56

copper: 63

tungsten: 184

ED = ejection energy (electron volts)

ED is approximately equal to twice the sublimation energy.

iron: 8

copper: 7

tungsten: 18

(e) Crystal and potential parameters

Symbols: CLATT, PMAXX, RELAX, XLMDA

CLATT = lattice constant (angstroms)

iron: 2.8665

copper: 3.6147

tungsten: 3.1650

PMAXX = potential cutoff (angstroms)

2 is used for iron and copper

RELAX = relaxation parameter (coordinate units squared)

The number of coordinate units an ejected atom must travel from its original lattice site in order to be considered displaced by CASCADE is $(RELAX)^{1\,2}$. RELAX = 5 is used for iron and copper.

XLMDA = 0 except when Bohr potential is used.

(f) Starting point for primary atom

Symbols: XO, YO, ZO

Coordinates are in angstroms. If a is the lattice constant in angstroms and (i,j,k) are the coordinates of the starting lattice site, then

$$XO = \frac{a}{2}\left(i-\frac{1}{2}\right)$$
$$YO = \frac{a}{2}\left(j-\frac{1}{2}\right)$$
$$ZO = \frac{a}{2}\left(k-\frac{1}{2}\right)$$

(g) Energy of primary atom

Symbol: EO (electron volts)

(h) Direction cosines of primary atom

Symbols: COSA, COSB, COSG

Cosines for the initial direction of motion. NMPO Program number 769 will select directions randomly from an isotropic distribution, and punch the appropriate data cards.

(i) End of record

(j) End of file

2. Minimum Data (CLUSTER)

(a) Number of intervals

Symbol: NTVAL

Number of intervals for the distance histograms. NTVAL ≤ 100

(b) Interval endpoints

Symbol: TVALS

In lattice coordinate units. There are NTVAL entries. TVALS(I) is the right-hand endpoint for the Ith interval.

(c) Random number generator

Symbol: RGEN (2 BCD words)

Octal bit pattern to initialize random number generation, specified in BCD.

(d) End of record

(e) End of file

Omission of the CLUSTER data will not cause the program to stop. Instead, it will use the following values:

NTVAL = 64

TVALS = 1,2,3,...,30,35,40,...,100,110,120,...,200,220,240,260,
280,300,350,400,450,500,600,700,800,900,1000.

RGEN = 235317167400

3. Deck Setup Example

The deck setup (Evendale) for a 5 keV copper run, based on the preceding two sections, is the following:

```
1ID
1STOP
1(5)A-6     REEL  XXXX  --  RING IN
1(5)B-4     REEL  3219  --  RING OUT
1(5)B=5     SCRATCH TAPE
1 SL(3) FORTRAN
*(5)XEQ

*(5)CHAIN (1,B2)
```

CASCADE binary deck (same for b.c.c. and f.c.c.)

*(5)CHAIN (1,B3)

EDIT binary deck (same for b.c.c. and f.c.c.)

*(5)CHAIN (2,B3)

CLUSTER binary deck (different for b.c.c. and f.c.c.)

```
*(5)DATA
5 ID1, 10, 5 KEV COPPER
5 ID2, 10, DIRECTION A1
5 TYPE 1, 2, COPPER
5 TYPE 2, 2, COPPER
5 TYPE 3, 2, COPPER
5 CRYSTL, 1, FCC
3 PCHG, 29, 29, 29, PMASS, 63, 63, 63, ED, 7, 7, 7,
3 CLATT, 3.6147, PMAXX, 2, RELAX, 5, XLMDA, 0,
3 XO, 362.3737, YO, 362.3737, ZO, 362.3737,
3 COSA, .58862761, COSB, .07788382, COSG, .86333006,
3 EO, 5000
=
8
4 NTVAL, 40,
3 TVALS, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20,
3 TVALS, 20 = ,21, 22, 23, 24, 25, 30, 35, 40, 45, 50, 60, 70, 80, 90, 100,
3 TVALS, 35 = ,150, 200, 250, 500, 1000,
5 RGEN, 2, 235217167400
=
8
```

4. Options

There are 17 optional deviations from the "minimum" or "standard" case. Instructions for specifying data for these options are given in this section.

(a) Change cases

One job may consist of an arbitrary number of cases. Each record of CASCADE data represents one case. All data carries over from one record to the next, except that which is explicitly changed.

CLUSTER reads only one record of data from tape 2, regardless of the number of cases. The defect lists will have been written on tape 7 by CASCADE, and CLUSTER reads and processes them successively until an end of file is reached.

(b) Print collision history

Control word: KPRINT (CASCADE data)

The results of each individual collision [ref [8], pp. 31-32, 50-52] are printed out, 50 collisions per page, if KPRINT is set equal to one.

(c) Run CASCADE alone

Control word: KLUSTR (CASCADE data)

If KLUSTR = 3, the program will rewind and unload tape 7 after CASCADE processing is complete, and call EXIT without loading CLUSTER.

(d) Run CLUSTER alone

Control word: KLUSTR (CASCADE data)

If KLUSTR = 1 in the first record of CASCADE data, control goes immediately to CLUSTER. Or else CLUSTER may be executed as a self-contained program without the presence of the other chain links.

(e) Potential data on cards

The potential data, or collision matrix [18] may be read in with the other data cards via tape 2, rather than on a binary data tape. The symbols are as follows:

NE: number of entries in energy table (NE $\leq$ 30)

NIP: number of entries in impact parameter table (NIP $\leq$ 30)

E: energy table (NE entries). The table is in ascending order, and must cover the range of possible energies. (electron volts). E(1) = 0. E(NE) $\geq$ EO.

P: impact parameter table (NIP entries). The table is in ascending order, and must cover the range of possible impact

parameters (in angstrom units). P(1) = 0. P(NIP) ≥ PMAXX

COSINE: scattering angle table. NE x NIP entries. COSINE (I,J) is the cosine of the center-of-mass scattering angle for a collision described by (P(I), E(J))

ETRA: transfer fraction table. NE x NIP entries. ETRA (I,J) is the fraction of energy transferred in a collision described by (P(I), E(J))

If the potential data is omitted from the data deck, it will be read from tape 10.

(f) Bohr potential

Symbol: XLMDA (CASCADE data)

If XLMDA ≠ 0, the program does not expect to find potential data as input. Instead, it computes the results of each collision using a hard-sphere approximation to a Bohr screened coulomb potential with screening parameter λ equal to XLMDA (ref [6], pp. 11-17).

XLMDA = 0 signals the program to use a collision matrix.

(g) Omit defect list printout - CASCADE

Control word: KPRINT (CASCADE data)

If KPRINT = 3, the defect list printed by CASCADE is omitted. In this case, the collision history is also omitted.

(h) Omit defect list printout - CLUSTER

Control word: KPRINT (CLUSTER data)

If KPRINT = 1, CLUSTER does not print out the defect list it uses for input.

(i) Trace primary atom only

Control word: KPRIM (CASCADE data)

If KPRIM = 1, only the collisions of the primary atom are traced. This option was provided in order to save machine time in channeling studies. Since in this case the damage pattern is not the object of interest, one should set KLUSTR = 3.

(j) Cut-off energy

Symbol: ECO (CASCADE data, 3 entries)

Atoms of the Jth kind (J = 1: type A, J = 2: type B, J = 3: primary) are traced until their energy falls below ECO (J) electron volts. If ECO (J) is not specified, it is set equal to ED (J).

(k) Subtraction energy

Symbol: ESUB (CASCADE data, 3 entries)

When energy E is transferred to an atom of the Jth kind, ejecting it from its lattice site (E > ED (J)), the energy of the ejected atom is taken to be E-ESUB (J). If ESUB (J) is unspecified, it is set equal to ED (J).

(l) Replacement collisions

Control word: KREPL (CASCADE data)

If KREPL = 1, replacement collisions are counted as such only when the moving atom and target atom are of different types. Otherwise, all replacement collisions are counted.

(m) Defect list input from cards - CLUSTER

Control word: KTAPE (CLUSTER data)

If KTAPE = 1, CLUSTER will read from tape 2 all the data normally on the defect list tape (section IV.4).

(n) Defect list input from specified records on tape 7 - CLUSTER

Symbols: NRECRD (one entry), KRECRD (NRECRD entries)

If NRECRD $\neq$ 0, CLUSTER will read NRECRD records from tape 7, NRECRD $\leq$ 10. The sequential numbers of the records (counting from the beginning of tape) are given by KRECRD (1-NRECRD).

If NRECRD = 0 or is unspecified, CLUSTER will process all records on tape 7 until an end of file is reached.

(o) SATURATION - first pass

Control word: KSATUR (CLUSTER data)

If KSATUR = 1, CLUSTER will write its input defect list, minus the unstable pairs, on tape 13. Tape 13 will then be available as the initial crystal state for a subsequent CASCADE run.

(p) SATURATION - nth pass, n $\geq$ 2

Control words: KSAT (SATURATION data and CASCADE data)
KSATUR (CLUSTER data)

If a cascade is to be run against a damage pattern computed earlier, the following changes should be made to the standard setup:

(i) The binary deck for the SATURATION link must be included physically preceding the CASCADE link. The control card is * CHAIN (2,B2).

(ii) One record of data for the SATURATION link precedes the data for the CASCADE link. This data includes KSAT = 1, and it includes identification ID1 (10 words) and ID2 (10 words), and a value for CRYSTL (BCC or FCC). Do not use an end-of-file (8) card to terminate the SATURATION data. The end-of-record (=) card is sufficient. The CASCADE data follows immediately.

(iii) Set KSAT = 1 in the CASCADE data and KSATUR = 1 in the CLUSTER data.

(iv) Mount the saturation tape (section IV.6) written by a previous job, as tape 13.

(q) SATURATION - nth pass, n ≥ 2, defect list from cards

If it is desired to specify a particular initial damage state which is not available on a binary tape, the setup is the same as in paragraph (p) with the following exceptions:

(i) KCAT = 3 in the SATURATION and CASCADE data.

(ii) Include NVAC, NINT, KVACX, KVACY, KVACZ, KINTX, KINTY, KINTZ with the SATURATION data.

VI PRINTOUT INTERPRETATION

1. CASCADE

The printout corresponding to the sample data of section V.3 is reproduced in Chapter VIII.

The first page of the CASCADE printout is a listing of the input data. The input values for the following parameters are listed under appropriate descriptive labels: CRYSTL, ID1 (1-10), ID2 (1-10), TYPE 1 (1-2), TYPE 2 (1-2), PMASS (1-2), PCHG (1-2), ED (1-2), TYPE 3 (1-2), PMASS (3), PCHG (3), EO, XO, YO, ZO, COSA, COSB, COSG, CLATT, XLMDA, PMAXX, RELAX.

THETA and PHI are the azimuthal and polar angles, respectively, corresponding to the given set of direction cosines. THETA = 0 lies in the XZ plane and PHI = 0 lies in the XY plane.

The values of control words are listed under the heading "output options." Control words are set equal to 2 by CASCADE unless specified in the input data. KPLAT and KRLAT are left over from an earlier version of the program, and have no meaning.

The collision history, if requested, appears next. It is omitted from this example, but an example and description appear in ref. [8]. If requested in this case, it would require 22 pages of printout.

The defect statistics appearing on page 2 are self-explanatory. Since the calculation is for a monatomic material, only the "TOTAL" row is relevant.

"Range" refers to the straight-line distance between the starting

point of the primary and its terminal position which, in this case, is a lattice site.

The lists of vacancies, interstitials, and replacements appear on the succeeding pages. The occurrence of two lists on each page reflects the provision for binary materials.

The primary knock-on energies are the energies (after ESUB is subtracted) of all atoms (there were 6 in this case) which were ejected by being struck by the primary atom.

The final page of the CASCADE printout is a message describing its normal termination. If there was a premature termination due to error, a message indicating that fact appears here.

2. CLUSTER

The first page of the CLUSTER printout is an input listing, including the CASCADE defect list, which is read from tape 7.

Page 2 is a list of the unstable Frenkel pairs and the type of each (section II.2). Except for the interstitials in types 0 and 1 pairs, the interstitials have now been assigned to lattice sites.

Page 3 gives the number of "stable" vacancies remaining after the unstable pairs have been deleted. The number of single vacancies, and the number of vacancies occurring in each size cluster from 2 on up is printed, and their coordinates are listed on page 4. Similar information about interstitials is given on page 5.

The remaining pages of the CLUSTER printout consist of distance tables,

the first two of which are reproduced.

The table labeled "distance between single vacancies" is interpreted in the following way:

There are 13 single vacancies, as seen from page 3. The number of distances between single vacancies is therefore $\frac{13!}{2!\ 11!} = 78$.

The average of these distances is labeled "average distance", and is given in three different systems of units. If one assigns to each of the 13 single vacancies a number equal to the distance from it to the nearest single vacancy, the average of these numbers is given under "average minimum distance."

Column I shows that 2 of the 78 distances lie between 2 and 3 units, 4 lie between 3 and 4, etc. Each interval is identified by its right-hand endpoint and includes the right-hand endpoint.

Column II shows the fraction of the total no. of distances in each interval, and Column III gives a cumulative distribution based on Column II.

Column IV normalizes the histogram to a unit volume. Since there were 4 distances in the interval (3,4], Column IV for the 4th interval is $\frac{4}{\frac{4}{3}\pi(4^3-3^3)} = .02581$. Column V is the same as Column IV, but in units of no./cubic coordinate unit.

Columns VI-X correspond to columns I-V respectively. The distribution refers to the 13 "minimum" distances rather than all 78 distances.

The table labeled "distance between single and divacancies" is similar, with the major differences arising from the fact that unlike defects are

being considered. The distribution of columns I-V refers to all single vacancy-divacancy distances, of which there are 13 x 3 = 39. The distribution of columns VI-X is the one which results from assigning to each of the 13 single vacancies a number representing the distance from it to the nearest divacancy.

In this case, the program prints 13 more similar distance tables, each for a different pair of defect types. These tables are interpreted in a manner similar to either the first or second table, according as the pair of types is like or unlike.

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ELASTIC COLLISION CASCADE -- FCC LATTICE

5 KEV COPPER
DIRECTION A5

CRYSTAL ATOMS

	1 COPPER	2 COPPER
MASS	63.	63.
CHARGE	29.	29.
EJECTION ENERGY	7.	7.

PRIMARY ATOM

COPPER MASS = 63. CHARGE = 29.

PRIMARY ATOM ENERGY

5000.0 ELECTRON VOLTS

TAKE-OFF POINT (ANGSTROMS)

X = 362.37370

Y = 362.37370

Z = 362.37370

TAKE-OFF DIRECTION

COS ALPHA = 0.58862761 COS BETA = 0.07788382 COS GAMMA = 0.80464381

THETA = 36.424130 PHI = 7.537266

LATTICE CONSTANT = 3.6147 ANGSTROMS

SCREENING PARAMETER = 0. POTENTIAL CUTOFF = 2.00 ANGSTROMS

RELAXATION DISTANCE (SQUARED) = 5.00 COORDINATE UNITS

OUTPUT OPTIONS

KLUSTR= 2 KPRIM= 2 KPRINT= 2 KRLAT= 2 KPLAT= 2 KREPL= 2

DEFECT STATISTICS

	INTERSTITIALS	VACANCIES	REPLACEMENTS
COPPER	44	53	62
COPPER	70	60	88
TOTAL	114	113	150

RANGE OF PRIMARY ATOM

12.62 ANGSTROMS

COORDINATES OF PRIMARY ATOM AT END OF CASCADE

203 204 206

COPPER VACANCIES

205 199 197	209 199 197	206 202 197	206 200 199	209 199 201	206 200 201	207 197 203	206 200 203
190 204 203	209 199 205	202 202 205	205 203 205	192 204 205	208 204 205	209 205 205	204 202 207
206 202 207	207 203 207	196 204 207	198 204 207	209 205 207	204 200 209	207 201 209	194 204 209
205 205 209	198 206 209	206 208 209	204 200 211	206 204 211	209 199 213	204 200 213	211 201 213
202 202 213	201 203 213	199 195 215	209 195 215	212 198 215	203 199 215	209 199 215	201 201 215
198 202 215	201 197 217	202 198 217	209 199 217	200 196 219	202 198 219	208 198 219	201 201 219
203 199 221	200 200 221	209 203 221	204 200 223	205 201 223			

COPPER VACANCIES

208 197 196	207 198 198	206 199 198	206 201 198	206 199 200	207 196 202	203 200 202	205 200 202
202 201 202	204 201 202	207 198 204	191 204 204	196 205 204	208 197 206	207 200 206	210 201 206
201 202 206	203 202 206	200 203 206	206 203 206	208 203 206	193 204 206	197 204 206	201 204 206
210 205 206	209 206 206	208 201 208	193 204 208	195 204 208	198 205 208	205 206 208	206 207 208
204 201 210	204 203 210	205 204 210	203 204 212	207 206 212	206 199 214	203 200 214	205 200 214
207 200 214	211 200 214	202 201 214	208 201 214	201 202 214	207 202 214	209 208 214	209 196 216
204 197 216	203 198 216	209 198 216	211 196 218	200 197 218	199 198 218	203 198 218	203 198 222
204 199 222	205 202 222	209 204 222	208 203 226				

COPPER INTERSTITIALS

206 197 195	202 199 197	210 201 197	206 205 197	206 205 199	208 204 200	192 204 202	195 205 202
195 207 202	207 194 203	204 196 204	207 199 204	207 203 204	204 201 205	199 204 207	204 206 207
208 207 207	209 208 207	207 197 208	198 204 210	212 204 210	204 198 211	207 203 211	208 203 211
205 201 212	197 205 212	196 195 213	199 202 213	209 202 213	197 200 215	203 200 215	213 200 215
198 203 215	200 202 216	210 196 217	200 196 218	198 196 220	212 196 220	197 200 221	203 197 222
209 206 223	208 204 224	208 204 228	204 200 232				

COPPER INTERSTITIALS

206 201 193	206 199 195	209 197 196	207 191 198	207 196 199	206 192 200	203 197 202	188 204 202
204 204 202	209 198 203	209 200 203	205 204 203	188 204 204	209 207 204	208 197 205	213 199 206
211 203 206	211 203 206	190 204 206	215 205 206	213 207 206	208 208 206	203 213 206	196 205 207
203 206 207	208 209 207	210 194 208	211 201 208	184 204 208	198 208 208	200 199 209	204 198 210
198 208 210	210 199 211	211 200 211	203 202 211	211 202 211	206 209 211	199 205 212	201 207 212
207 207 212	211 196 213	193 204 213	203 204 213	208 192 214	204 194 214	211 195 214	203 197 214
205 203 214	208 208 214	210 210 214	195 204 215	200 192 216	203 193 216	207 193 216	209 197 215
201 201 216	198 196 218	206 196 218	210 196 218	196 198 218	201 203 218	210 201 219	200 194 220
207 198 221	206 198 222	207 201 222	205 205 222	203 198 225	209 201 226		

COPPER REPLACEMENTS

203 199 197	210 200 197	206 204 197	206 202 199	206 204 199	208 204 201	209 198 202	208 201 202
189 204 202	207 195 203	192 204 203	208 204 203	209 200 204	209 206 204	204 202 205	208 202 205
204 197 206	212 207 206	200 204 207	209 207 207	204 199 208	201 200 208	208 203 208	210 205 208
207 208 208	193 204 209	206 201 210	208 201 210	193 204 210	195 204 210	198 207 210	206 209 210
204 198 211	204 198 211	207 203 211	210 199 212	203 202 212	211 202 212	200 205 212	208 193 214
198 195 214	210 195 214	212 197 214	203 198 214	212 200 215	197 201 215	200 193 216	209 200 218
201 202 218	199 197 219	201 197 219	200 195 220	207 198 220	198 200 221	206 201 222	208 204 223
204 200 225	207 203 225	204 200 227	208 204 227	204 200 229	204 200 231		

COPPER REPLACEMENTS

206 201 194	207 197 195	209 198 196	206 199 196	206 201 196	207 192 198	207 194 198	207 196 198
206 193 200	206 195 200	207 196 200	206 197 200	203 198 202	204 203 202	208 202 203	195 205 203
196 206 203	208 197 204	189 204 204	205 204 204	204 196 205	207 199 205	212 199 206	211 200 205
210 203 206	211 203 206	191 204 206	202 205 206	212 205 206	214 205 206	203 206 206	208 207 205
203 208 206	203 210 206	203 212 206	207 197 207	204 198 207	201 201 207	204 206 207	207 207 207
210 195 208	210 201 208	185 204 208	187 204 209	189 204 208	191 204 208	198 207 208	211 205 209
204 199 210	195 204 210	205 201 211	208 202 211	196 204 211	211 200 212	193 204 212	195 204 212
202 205 212	201 206 212	197 195 213	200 202 213	208 202 213	205 194 214	206 195 214	206 197 214
210 201 214	206 203 214	195 204 214	210 209 214	208 194 215	204 200 215	200 202 215	203 194 215
207 194 216	203 196 216	206 197 216	208 197 216	210 196 217	199 196 218	205 196 218	204 197 218
210 197 218	197 198 218	212 196 219	205 198 222	205 204 222	209 205 223	203 198 224	209 202 226

PRIMARY KNOCK-ON ENERGIES (EV)

COPPER 2	COPPER 4
10.44	4.60
621.61	74.60
0.	1093.89
0.	345.56

NUMBER OF COLLISIONS RECORDED = 1080

VOLUME OF DAMAGED REGION = 3.892+04 C.A.

MAXIMUM PERMITTED VOLUME = 5.658+05 C.A.

CASCADE PROGRAM RAN ALL CASES TO COMPLETION

WILL NOW WRITE END OF FILE ON 7, REWIND, AND CALL CLUSTER

FCC VACANCY CLUSTER SIZE DISTRIBUTION AND DEPLOYMENT PROGRAM, NMP779

5 KEV COPPER
DIRECTION A5

LATTICE CONSTANT = 3.6147000+00
RANDOM NUMBER GENERATOR = 235217167400
CONTROL WORDS - KTAPE= 0, KPRINT= 0, KODE= 0, KRECRD= 0,

DEFECT SITES, LIST 1

VACANCIES - 53			INTERSTITIALS - 44		
205	199	197	206	197	195
209	199	197	202	199	197
206	202	197	210	201	197
206	200	199	206	205	197
209	199	201	206	205	199
206	200	201	208	204	200
207	197	203	192	204	202
206	200	203	195	205	202
190	204	203	195	207	202
209	199	205	207	194	203
202	202	205	204	196	204
205	203	205	207	199	204
192	204	205	207	203	204
208	204	205	204	201	205
209	205	205	199	204	207
204	202	207	204	206	207
206	202	207	208	207	207
207	203	207	209	208	207
196	204	207	207	197	208
198	204	207	198	204	210
209	205	207	212	204	210
204	200	209	204	198	211
207	201	209	207	203	211
194	204	209	208	203	211
205	205	209	205	201	212
198	206	209	197	205	212
206	208	209	196	195	213
204	200	211	199	202	213
206	204	211	209	202	213
209	199	213	197	200	215
204	200	213	203	200	215
211	201	213	213	200	215
202	202	213	198	203	215
201	203	213	200	202	216
199	195	215	210	196	217
209	195	215	200	196	218
212	198	215	198	196	220
203	199	215	212	196	220
209	199	215	197	200	221
201	201	215	203	197	222
198	202	215	209	206	223
201	197	217	208	204	224
202	198	217	208	204	228
209	199	217	204	200	232
200	196	219	0	0	0
202	198	219	0	0	0
208	198	219	0	0	0
201	201	219	0	0	0
203	199	221	0	0	0
200	200	221	0	0	0
209	203	221	0	0	0
204	200	223	0	0	0

DEFECT SITES, LIST 2

VACANCIES - 60			INTERSTITIALS - 70		
208	197	196	206	201	193
207	198	198	206	199	195
206	199	198	209	197	196
206	201	198	207	191	198
206	199	200	207	196	199
207	196	202	206	192	200
203	200	202	203	197	202
205	200	202	188	204	202
202	201	202	204	204	202
204	201	202	209	198	203
207	198	204	209	200	203
191	204	204	205	204	203
196	205	204	188	204	204
208	197	206	209	207	204
207	200	206	208	197	205
210	201	206	213	199	206
201	202	206	211	203	206
203	202	206	211	203	206
200	203	206	190	204	206
206	203	206	215	205	206
208	203	206	213	207	206
193	204	206	208	208	206
197	204	206	203	213	206
201	204	206	196	205	207
210	205	206	203	206	207
209	206	206	208	209	207
208	201	208	210	194	208
193	204	208	211	201	208
195	204	208	184	204	208
198	205	208	198	208	208
205	206	208	200	199	209
206	207	208	204	198	210
204	201	210	198	208	210
204	203	210	210	199	211
205	204	210	211	200	211
203	204	212	203	202	211
207	206	212	211	202	211
206	199	214	206	209	211
203	200	214	199	205	212
205	200	214	201	207	212
207	200	214	207	207	212
211	200	214	211	196	213
202	201	214	193	204	213
208	201	214	203	204	213
201	202	214	208	192	214
207	202	214	204	194	214
209	208	214	211	195	214
209	196	216	203	197	214
204	197	216	205	203	214
203	198	216	208	208	214
209	198	216	210	210	214
211	196	218	195	204	215

205	201	223	0	0	0	200	197	218	200	192	216
0	0	0	0	0	0	199	198	218	203	193	216
0	0	0	0	0	0	203	198	218	207	193	216
0	0	0	0	0	0	203	198	222	209	197	216
0	0	0	0	0	0	204	199	222	201	201	216
0	0	0	0	0	0	205	202	222	198	196	218
0	0	0	0	0	0	209	204	222	206	196	218
0	0	0	0	0	0	208	203	226	210	196	218
0	0	0	0	0	0	0	0	0	196	198	218
0	0	0	0	0	0	0	0	0	201	203	218
0	0	0	0	0	0	0	0	0	210	201	219
0	0	0	0	0	0	0	0	0	200	194	220
0	0	0	0	0	0	0	0	0	207	198	221
0	0	0	0	0	0	0	0	0	206	198	222
0	0	0	0	0	0	0	0	0	207	201	222
0	0	0	0	0	0	0	0	0	205	205	222
0	0	0	0	0	0	0	0	0	203	198	225
0	0	0	0	0	0	0	0	0	209	201	226

FCC VACANCY CLUSTER SIZE DISTRIBUTION AND DEPLOYMENT PROGRAM, NMP779

5 KEV COPPER
DIRECTION A5

UNSTABLE FRENKEL PAIRS - 52

VACANCIES			INTERSTITIALS			TYPE	VACANCIES			INTERSTITIALS			TYPE
207	198	204	207	199	204	1	198	204	207	199	204	207	1
203	199	215	203	200	215	1	198	202	215	198	203	215	1
200	196	219	200	196	218	1	203	198	222	203	197	222	1
208	197	196	209	197	196	1	208	197	206	208	197	205	1
196	204	207	196	205	207	1	207	206	212	207	207	212	1
203	204	212	203	204	213	1	209	208	214	208	208	214	1
209	196	216	209	197	216	1	201	201	215	201	201	216	1
211	196	218	210	196	218	1	209	199	197	210	200	197	2
190	204	203	191	204	202	2	205	206	208	204	206	207	2
209	206	206	209	207	207	2	198	206	209	198	205	210	2
206	204	211	207	203	211	2	208	201	214	209	201	213	2
209	204	222	209	205	223	2	205	203	205	205	204	204	2
210	205	206	211	204	206	2	204	201	210	204	202	211	2
204	200	211	204	198	211	3	204	201	202	204	203	202	3
209	199	201	209	199	203	3	206	200	203	208	200	203	3
210	201	206	210	203	206	3	211	201	213	211	201	211	3
205	200	214	205	202	214	3	196	205	204	194	205	202	4
207	196	202	207	194	204	4	202	202	205	204	200	205	4
206	208	209	208	208	207	4	205	204	210	205	202	212	4
201	202	214	199	202	212	4	211	200	214	213	200	216	4
208	203	226	208	205	224	4	206	207	208	208	207	206	4
205	205	209	203	205	207	4	209	195	215	211	195	213	4
204	197	216	206	197	218	4	206	201	198	206	198	195	5
207	200	206	207	203	203	5	199	195	215	196	195	212	5
206	202	197	206	199	194	5	207	200	214	210	200	211	5
207	202	214	210	202	211	5	208	198	219	208	201	222	5

FCC VACANCY CLUSTER SIZE DISTRIBUTION AND DEPLOYMENT PROGRAM, NMP779

5 KEV COPPER
DIRECTION A5

NUMBER OF INPUT VACANCIES	113
NUMBER OF UNSTABLE PAIRS	52
NUMBER OF STABLE VACANCIES	61

TYPE OF CLUSTER	NUMBER OF CLUSTERS
1-VACANCY	13
2-VACANCY	3
3-VACANCY	4
5-VACANCY	2
6-VACANCY	1
7-VACANCY	2

SINGLE VACANCIES

207	197	203	209	199	205	209	205	207	204	200	209	209	199	213
212	198	215	201	201	219	200	200	221	209	203	221	197	204	206
198	205	208	204	203	210	206	199	214						

VACANCY CLUSTERS

7-VACANCY CLUSTER	205	199	197
	206	200	199
	206	200	201
	206	199	198
	207	198	198
	206	199	200
	205	200	202
3-VACANCY CLUSTER	192	204	205
	191	204	204
	193	204	206
6-VACANCY CLUSTER	208	204	205
	209	205	205
	207	203	207
	206	202	207
	208	203	206
	206	203	206
2-VACANCY CLUSTER	204	202	207
	203	202	206
2-VACANCY CLUSTER	207	201	209
	208	201	208
3-VACANCY CLUSTER	194	204	209
	193	204	208
	195	204	208
5-VACANCY CLUSTER	204	200	213
	202	202	213
	201	203	213
	203	200	214
	202	201	214
3-VACANCY CLUSTER	209	199	215
	209	199	217

	209	198	216
7-VACANCY CLUSTER	201	197	217
	202	198	217
	202	198	219
	200	197	218
	203	198	216
	203	198	218
	199	198	218
5-VACANCY CLUSTER	203	199	221
	204	200	223
	205	201	223
	204	199	222
	205	202	222
2-VACANCY CLUSTER	203	200	202
	202	201	202
3-VACANCY CLUSTER	201	202	206
	200	203	206
	201	204	206

FCC VACANCY CLUSTER SIZE DISTRIBUTION AND DEPLOYMENT PROGRAM, NMP779

5 KEV COPPER
DIRECTION A5

NUMBER OF INPUT INTERSTITIALS 114
NUMBER OF UNSTABLE PAIRS 52
NUMBER OF STABLE INTERSTITIALS 62

TYPE OF CLUSTER	NUMBER OF CLUSTERS
1-INTERSTITIAL	52
2-INTERSTITIAL	5

SINGLE INTERSTITIALS

202	199	196	206	206	197	207	205	199	209	204	200	194	207	202
204	196	205	207	197	207	212	203	210	209	203	211	198	200	215
200	202	217	210	196	217	198	195	220	212	197	220	197	200	220
208	204	229	204	200	231	206	202	193	207	191	197	206	196	199
207	192	200	203	196	202	208	207	204	213	199	205	190	203	206
215	204	206	213	207	207	203	213	207	209	209	207	211	194	208
211	200	208	184	204	209	197	208	208	199	199	209	205	198	210
198	209	210	206	209	212	201	206	212	194	204	213	212	195	214
203	197	213	210	209	214	195	204	216	199	192	216	198	196	217
196	197	218	201	204	218	210	202	219	200	194	219	204	205	222
203	197	225	209	200	226									

INTERSTITIAL CLUSTERS

2-INTERSTITIAL CLUSTER	197	205	211
	198	205	212
2-INTERSTITIAL CLUSTER	188	204	203
	188	205	204
2-INTERSTITIAL CLUSTER	208	192	215
	207	193	215
2-INTERSTITIAL CLUSTER	204	194	215
	204	193	216
2-INTERSTITIAL CLUSTER	207	199	221
	207	198	222

FCC VACANCY CLUSTER SIZE DISTRIBUTION AND DEPLOYMENT PROGRAM, NMP779

5 KEV COPPER
DIRECTION A5

DISTANCE BETWEEN SINGLE VACANCIES

	COORD. UNITS	ANGSTROMS	LATTICE CONSTANTS
AVERAGE DISTANCE	1.0799+01	1.9518+01	5.3996+00
AVERAGE MINIMUM DISTANCE	3.6652+00	6.6243+00	1.8326+00

TOTAL OF COLUMN I 1.8000000+01
TOTAL OF COLUMN IV 13

INTERVAL	I	II	III	IV	V	VI	VII	VIII	IX	X
1.0	0	0.	0.	0.	0.	0	0.	0.	0.	0.
2.0	0	0.	0.	0.	0.	0	0.	0.	0.	0.
3.0	2	0.2564-01	0.2564-01	0.2513-01	0.4257-02	4	0.3077-00	0.3077-00	0.5026-01	0.8513-02
4.0	4	0.5128-01	0.7692-01	0.2581-01	0.4372-02	7	0.5385+00	0.8462+00	0.4517-01	0.7650-02
5.0	0	0.	0.7692-01	0.	0.	0	0.	0.8462+00	0.	0.
6.0	2	0.2564-01	0.1026-00	0.5247-02	0.8887-03	0	0.	0.8462+00	0.	0.
7.0	6	0.7692-01	0.1795-00	0.1128-01	0.1910-02	1	0.7692-01	0.9231+00	0.1880-02	0.3184-03
8.0	6	0.7692-01	0.2564-00	0.8476-02	0.1436-02	0	0.	0.9231+00	0.	0.
9.0	8	0.1026-00	0.3590-00	0.8801-02	0.1491-02	1	0.7692-01	1.0000+00	0.1100-02	0.1863-03
10.0	7	0.8974-01	0.4487-00	0.6167-02	0.1045-02	0	0.	1.0000+00	0.	0.
11.0	6	0.7692-01	0.5256+00	0.4327-02	0.7330-03	0	0.	1.0000+00	0.	0.
12.0	4	0.5128-01	0.5769+00	0.2405-02	0.4074-03	0	0.	1.0000+00	0.	0.
13.0	9	0.1154-00	0.6923+00	0.4581-02	0.7760-03	0	0.	1.0000+00	0.	0.
14.0	8	0.1026-00	0.7949+00	0.3492-02	0.5914-03	0	0.	1.0000+00	0.	0.
15.0	4	0.5128-01	0.8462+00	0.1513-02	0.2563-03	0	0.	1.0000+00	0.	0.
16.0	1	0.1282-01	0.8590+00	0.3311-03	0.5609-04	0	0.	1.0000+00	0.	0.
17.0	2	0.2564-01	0.8846+00	0.5844-03	0.9899-04	0	0.	1.0000+00	0.	0.
18.0	4	0.5128-01	0.9359+00	0.1039-02	0.1760-03	0	0.	1.0000+00	0.	0.
19.0	2	0.2564-01	0.9615+00	0.4649-03	0.7875-04	0	0.	1.0000+00	0.	0.
20.0	3	0.3846-01	1.0000+00	0.6277-03	0.1063-03	0	0.	1.0000+00	0.	0.
21.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
22.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
23.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
24.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
25.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
30.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
35.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
40.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
45.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
50.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
60.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
70.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
80.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
90.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
100.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
150.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
200.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
250.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
500.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
1000.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
INFINITY	0	0.	1.0000+00	---	---	0	0.	1.0000+00	---	---

FCC VACANCY CLUSTER SIZE DISTRIBUTION AND DEPLOYMENT PROGRAM, NMP779

5 KEV COPPER
DIRECTION A5

DISTANCE BETWEEN SINGLE AND DIVACANCIES

	COORD. UNITS	ANGSTROMS	LATTICE CONSTANTS
AVERAGE DISTANCE	9.5061+00	1.7181+01	4.7530+00
AVERAGE MINIMUM DISTANCE	7.2420+00	1.3089+01	3.6210+00

TOTAL OF COLUMN I 3.9000000+01
TOTAL OF COLUMN IV 13

INTERVAL	I	II	III	IV	V	VI	VII	VIII	IX	X
1.0	0	0.	0.	0.	0.	0	0.	0.	0.	0.
2.0	0	0.	0.	0.	0.	0	0.	0.	0.	0.
3.0	0	0.	0.	0.	0.	0	0.	0.	0.	0.
4.0	3	0.7692-01	0.7692-01	0.1936-01	0.3279-02	2	0.1538-00	0.1538-00	0.1290-01	0.2186-02
5.0	3	0.7692-01	0.1538-00	0.1174-01	0.1989-02	2	0.1538-00	0.3077-00	0.7827-02	0.1326-02
6.0	2	0.5128-01	0.2051-00	0.5247-02	0.8887-03	2	0.1538-00	0.4615-00	0.5247-02	0.8887-03
7.0	6	0.1538-00	0.3590-00	0.1128-01	0.1910-02	3	0.2308-00	0.6923+00	0.5639-02	0.9552-03
8.0	4	0.1026-00	0.4615-00	0.5650-02	0.9571-03	0	0.	0.6923+00	0.	0.
9.0	4	0.1026-00	0.5641+00	0.4401-02	0.7454-03	1	0.7692-01	0.7692+00	0.1100-02	0.1863-03
10.0	2	0.5128-01	0.6154+00	0.1762-02	0.2984-03	0	0.	0.7692+00	0.	0.
11.0	1	0.2564-01	0.6410+00	0.7212-03	0.1222-03	0	0.	0.7692+00	0.	0.
12.0	1	0.2564-01	0.6667+00	0.6013-03	0.1019-03	0	0.	0.7692+00	0.	0.
13.0	6	0.1538-00	0.8205+00	0.3054-02	0.5173-03	2	0.1538-00	0.9231+00	0.1018-02	0.1724-03
14.0	0	0.	0.8205+00	0.	0.	0	0.	0.9231+00	0.	0.
15.0	1	0.2564-01	0.8462+00	0.3783-03	0.6408-04	1	0.7692-01	1.0000+00	0.3783-03	0.6408-04
16.0	2	0.5128-01	0.8974+00	0.6622-03	0.1122-03	0	0.	1.0000+00	0.	0.
17.0	1	0.2564-01	0.9231+00	0.2922-03	0.4950-04	0	0.	1.0000+00	0.	0.
18.0	1	0.2564-01	0.9487+00	0.2598-03	0.4400-04	0	0.	1.0000+00	0.	0.
19.0	0	0.	0.9487+00	0.	0.	0	0.	1.0000+00	0.	0.
20.0	1	0.2564-01	0.9744+00	0.2092-03	0.3544-04	0	0.	1.0000+00	0.	0.
21.0	1	0.2564-01	1.0000+00	0.1893-03	0.3207-04	0	0.	1.0000+00	0.	0.
22.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
23.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
24.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
25.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
30.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
35.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
40.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
45.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
50.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
60.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
70.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
80.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
90.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
100.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
150.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
200.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
250.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
500.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
1000.0	0	0.	1.0000+00	0.	0.	0	0.	1.0000+00	0.	0.
INFINITY	0	0.	1.0000+00	---	---	0	0.	1.0000+00	---	---

ADVANCED TECHNOLOGY SERVICES

GENERAL ELECTRIC